UNIFORM ELECTRON GAS FROM TWO-PARTICLE WAVEFUNCTIONS

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1. INTRODUCTION

A common approach to the many-electron problem (atoms, molecules and solids) is its transformation into a fewer-particle problem. In Density Functional Theory[1,2] (DFT) one rewrites the ground-state energy of a many-electron system as a functional of just the one-electron density $n(\mathbf{r})$, the diagonal part of the one-particle reduced density matrix. In recent years, much attention has been devoted to approaches which rewrite the system energy as a functional of the one- or the two-particle reduced density matrix.[3–9] With respect to DFT, these approaches have the advantage that the kinetic energy functional is known and that they provide more information about the many-body wavefunction. In this contest, the relevance of two-electron wavefunctions (geminals) has been pointed out: the use of an antisymmetrized geminal power wavefunction, i.e., a many-body wavefunction built in terms of geminals with the correct symmetry under particle permutation, provides the basis for a formally correct one-particle reduced density matrix functional theory.[3]

With these concepts in mind, it is of great interest to start with a simple many-body system, the uniform electron gas, a limit which should be recovered by any approximate approach to the many-electron problem of nonuniform density. A more detailed discussion about reduced-density matrix functionals applied to the uniform electron gas can be found in Refs. 7,10–12. In this paper, an approximation for the unknown two-electron wavefunctions (geminals) of the uniform electron gas is found, starting from the effective screened Coulomb potential proposed by Overhauser.[13] The short-range part (small electron-electron distances) of the corresponding pair density is found to be in accurate agreement with the newest Quantum Monte

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Carlo data.[16] This means that the short-range part of these geminals is reliable and could serve as a useful term of comparison for other two-electron approaches to the uniform electron gas.[7, 10–12]

2. ELECTRON PAIR-DENSITIES, ETC.

Given an N-electron wavefunction $\Psi(\mathbf{r}_1\sigma_1, ...\mathbf{r}_N\sigma_N)$, we define the pair density

$$\rho_2(\mathbf{r}, \mathbf{r}') = N(N-1) \sum_{\sigma_i=1}^{N} \int \prod_{j=3}^{N} d\mathbf{r}_j |\Psi(\mathbf{r}\sigma_1, \mathbf{r}'\sigma_2, ...\mathbf{r}_N\sigma_N)|^2, \tag{1}$$

the one-particle density matrix

$$\rho_1(\mathbf{r}, \mathbf{r}') = N \sum_{\sigma_i=1}^{N} \int \Psi^*(\mathbf{r}\sigma_1, \mathbf{r}_2\sigma_2, ...\mathbf{r}_N\sigma_N)\Psi(\mathbf{r}'\sigma_1, \mathbf{r}_2\sigma_2, ...\mathbf{r}_N\sigma_N)d\mathbf{r}_2...d\mathbf{r}_N, \tag{2}$$

and the one-electron density

$$n(\mathbf{r}) = \rho_1(\mathbf{r}, \mathbf{r}) = \frac{1}{N-1} \int d\mathbf{r}' \rho_2(\mathbf{r}, \mathbf{r}'). \tag{3}$$

While $n(\mathbf{r})d\mathbf{r}$ is the probability of finding an electron in $d\mathbf{r}$, $\rho_2(\mathbf{r}, \mathbf{r}')d\mathbf{r}d\mathbf{r}'$ is the probability of finding one electron in $d\mathbf{r}$ and another in $d\mathbf{r}'$. We also define the pair-distribution function $g(\mathbf{r}, \mathbf{r}')$:

$$\rho_2(\mathbf{r}, \mathbf{r}') = n(\mathbf{r})n(\mathbf{r}')g(\mathbf{r}, \mathbf{r}'). \tag{4}$$

By integrating Eq. (1) over $\mathbf{r}'$, we find that

$$\int d\mathbf{r}'n(\mathbf{r}') \left[g(\mathbf{r}, \mathbf{r}') - 1\right] = -1. \tag{5}$$

In other words, the density $n(\mathbf{r}')[g(\mathbf{r}, \mathbf{r}')-1]$ of the exchange-correlation hole around an electron at $\mathbf{r}$ represents a deficit of one electron.

3. UNIFORM ELECTRON GAS (JELLIUM)

The three-dimensional jellium model consists of N electrons enclosed in a box of volume V (periodically repeated in space) in the presence of a neutralizing background of uniform positive charge density $n^+ = N/V$. The non relativistic jellium is thus governed by the hamiltonian (in Hartree atomic units):

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2} + \frac{1}{2} \sum_{i \neq j=1}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \Lambda, \tag{6}$$

where Λ represents the effect of the background. The hamiltonian of Eq. (6) describes a model solid whose positive ionic charges are smeared throughout the whole crystal volume to yield a shapeless, uniform positive background (whence the nickname of jellium). When studying this model, one is usually interested in its macroscopic properties, i.e., the thermodynamic limit ($N, V \to \infty$ keeping $n = N/V$ constant) of its extensive physical quantities per particle or per volume. Two numbers are enough to describe its zero-temperature phase diagram, namely, the one-electron density $n = N/V$ and the spin polarization $\zeta = |N_\uparrow - N_\downarrow|/N$, where $N_{\uparrow(\downarrow)}$ is the number of spin-up (down) electrons ($N = N_\uparrow + N_\downarrow$). Instead of the particle density n, it is often convenient to use the Wigner-Seitz radius r_s (in units of the Bohr radius) given by $r_s = \left(\frac{4\pi}{3} n\right)^{-1/3}$; it is also useful to define the Fermi wavevector k_F, simply related to the r_s parameter by $k_F = \left(3\pi^2 n\right)^{1/3} = (\frac{9\pi}{4})^{1/3}\frac{1}{r_s}$.

Beeing the system homogeneous and isotropic, the pair-distribution function only depends on $r = |\mathbf{r}_1 - \mathbf{r}_2|$, and parametrically on r_s and ζ.

4. JELLIUM FROM TWO-ELECTRON WAVEFUNCTIONS

The pair-distribution function of jellium can be built starting from two-electron wavefunctions.[13, 14] We first rewrite the non-interacting gas (ideal Fermi gas) in terms of two-electron wavefunctions. This first step can seem redundant, since the ideal gas can be written in terms of one-electron wavefunctions, as a Slater determinant of plane waves. However, treating first the ideal gas is essential to set the proper normalization. The two-electron wavefunctions for the interacting gas, in fact, are found by solving a scattering problem in an effective potential, with the normalization condition that the ideal gas is recovered when the potential is set to zero. In this paper, only the $\zeta = 0$ case is analysed. For the generalization to the $\zeta \neq 0$ gas see Ref. 14.

4.1. Ideal Fermi gas

If we select a pair of electrons at random in the spin-unpolarized uniform gas, there is one chance in four that they will be in the singlet state, $\uparrow\downarrow - \downarrow\uparrow$, and three chances in four that they will be in one of the triplet states, $\uparrow\uparrow$, $\downarrow\downarrow$, $\uparrow\downarrow + \downarrow\uparrow$. In the case of no electron-electron interaction, the corresponding two-electron spatial wavefunctions can be rewritten in the center-of-mass reference system as

$$\Psi(\mathbf{r}, \mathbf{R}) = \frac{1}{\sqrt{2}} e^{i\,\mathbf{K}\cdot\mathbf{R}} \left(e^{i\,\mathbf{k}\cdot\mathbf{r}} \pm e^{-i\,\mathbf{k}\cdot\mathbf{r}}\right), \tag{7}$$

where "+"is for the singlet state and "−" is for the triplet state, and

$$\mathbf{R} = \tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2), \qquad \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1, \qquad \mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2, \qquad \mathbf{k} = \tfrac{1}{2}(\mathbf{k}_2 - \mathbf{k}_1). \tag{8}$$

Beeing the system isotropic, it is convenient to expand the plane waves into spherical harmonics

$$e^{i\,\mathbf{k}\cdot\mathbf{r}} = \sum_{\ell=0}^{\infty}(2\ell + 1)\, i^\ell\, P_\ell(\cos\theta)\, j_\ell(k\,r), \tag{9}$$

where P_ℓ are Legendre polynomials and j_ℓ are spherical Bessel functions. Then

$$\Psi_{\text{singlet}}(\mathbf{r}, \mathbf{R}) \;=\; \sqrt{2}\,e^{i\,\mathbf{K}\cdot\mathbf{R}} \sum_{\substack{\ell=0 \\ \text{even } \ell}}^{\infty} (2\ell+1)\,i^\ell\,P_\ell(\cos\theta)\,j_\ell(k\,r) \tag{10}$$

$$\Psi_{\text{triplet}}(\mathbf{r}, \mathbf{R}) \;=\; \sqrt{2}\,e^{i\,\mathbf{K}\cdot\mathbf{R}} \sum_{\substack{\ell=1 \\ \text{odd } \ell}}^{\infty} (2\ell+1)\,i^\ell\,P_\ell(\cos\theta)\,j_\ell(k\,r). \tag{11}$$

The pair-distribution function can be obtained by Ψ_{singlet} and Ψ_{triplet} by giving them the proper weight,

$$g(r) = \tfrac{1}{4}\langle|\Psi_{\text{singlet}}(\mathbf{r})|^2\rangle + \tfrac{3}{4}\langle|\Psi_{\text{triplet}}(\mathbf{r})|^2\rangle, \tag{12}$$

and by considering that in the uniform electron gas there is a probability $p(k)$ that two electrons have a given relative momentum $k = \frac{1}{2}|\mathbf{k}_1 - \mathbf{k}_2|$. In Eq. (12) the symbol $\langle\rangle$ means, in fact, that an average over $p(k)$ and over the solid angle has to be performed. If one is interested in the spin-resolved pair-distribution functions, $g_{\uparrow\uparrow}(r)$ and $g_{\uparrow\downarrow}(r)$, corresponding to parallel- and antiparallel-spin interactions, and such that for the unpolarized gas

$$g = \tfrac{1}{2}(g_{\uparrow\uparrow} + g_{\uparrow\downarrow}), \tag{13}$$

one has to consider that $\frac{1}{3}$ of the triplet state $(\uparrow\downarrow + \downarrow\uparrow)$ contributes to the antiparallel-spin correlations and $\frac{2}{3}$ of it $(\uparrow\uparrow$ and $\downarrow\downarrow)$ to the parallel-spin correlations. So, we have

$$g_{\uparrow\downarrow}(r) \;=\; \tfrac{1}{2}\langle|\Psi_{\text{singlet}}(\mathbf{r})|^2\rangle + \tfrac{1}{2}\langle|\Psi_{\text{triplet}}(\mathbf{r})|^2\rangle \tag{14}$$

$$g_{\uparrow\uparrow}(r) \;=\; \langle|\Psi_{\text{triplet}}(\mathbf{r})|^2\rangle, \tag{15}$$

where $\langle\rangle$ denotes again average over $p(k)$ and over the solid angle. Performing the spherical average over the solid angle, we obtain:

$$g_{\uparrow\downarrow}(r) \;=\; \sum_{\ell=0}^{\infty} (2\ell+1)\langle j_\ell^2(k\,r)\rangle \tag{16}$$

$$g_{\uparrow\uparrow}(r) \;=\; 2\sum_{\substack{\ell=1 \\ \text{odd } \ell}}^{\infty} (2\ell+1)\langle j_\ell^2(k\,r)\rangle. \tag{17}$$

Equation (16) immediately gives the exact result for a noninteracting gas, i.e., $g_{\uparrow\downarrow}(r) = 1$ for each r. To obtain the noninteracting $g_{\uparrow\uparrow}(r)$ from Eq. (17), we need to average over k. In the noninteracting electron gas, the probability distribution $p(k)$ for $k = \frac{1}{2}|\mathbf{k}_2 - \mathbf{k}_1|$ can be obtained geometrically by considering two three-dimensional vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ with $0 \leq |\mathbf{k}_{1(2)}| \leq k_F$, where k_F is the Fermi wavevector. The probability $p(k)$ is then

$$p(k) = 24\frac{k^2}{k_F^3} - 36\frac{k^3}{k_F^4} + 12\frac{k^5}{k_F^6}, \tag{18}$$

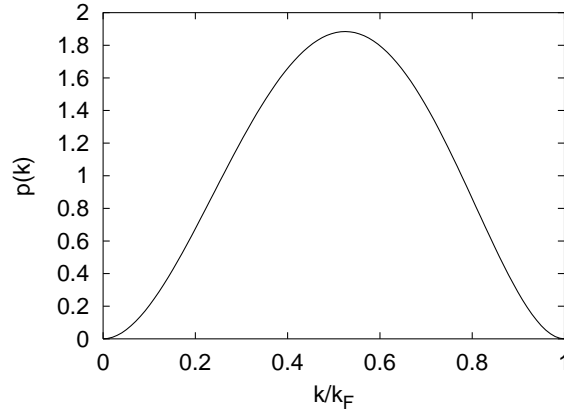with k ranging from 0 to k_F (see Fig. 1). By using two known series which involve

Figure 1: Relative-momentum ($k = \frac{1}{2}|\mathbf{k}_2 - \mathbf{k}_1|$) probability distribution $p(k)$ for the noninteracting gas.

j_ℓ^2,

$$\sum_{\ell=0}^{\infty}(2\ell+1)j_\ell^2(x) = 1 \qquad \sum_{\ell=0}^{\infty}(-1)^\ell(2\ell+1)j_\ell^2(x) = \frac{\sin(2x)}{2x}, \qquad (19)$$

we can rewrite $g_{\uparrow\uparrow}$ as

$$g_{\uparrow\uparrow}(r) = \sum_{\ell=0}^{\infty}(2\ell+1)\langle j_\ell^2(k\,r)\rangle - \sum_{\ell=0}^{\infty}(-1)^\ell(2\ell+1)\langle j_\ell^2(k\,r)\rangle = \left\langle 1 - \frac{\sin(2kr)}{2kr}\right\rangle. \tag{20}$$

This means:

$$g_{\uparrow\uparrow}(r) = \int_0^{k_F}\left[1 - \frac{\sin(2kr)}{2kr}\right]\left(24\frac{k^2}{k_F^3} - 36\frac{k^3}{k_F^4} + 12\frac{k^5}{k_F^6}\right)\,dk. \tag{21}$$

Performing this integral gives the known Hartree-Fock (noninteracting) $g_{\uparrow\uparrow}$,

$$g_{\uparrow\uparrow}^{\text{HF}} = 1 - 9\left[\frac{\sin(k_F r) - k_F r\cos(k_F r)}{(k_F r)^3}\right]^2. \tag{22}$$

Numerically, in the range $0 \leq k_F r \leq 6$ and with a truncation of the infinite sum over ℓ at $\ell_{\max} = 7$, Eq. (17) reproduces the exact Eq. (22) within an accuracy of 10^{-6}. When the scaled variable $k_F r$ (or equivalently r/r_s) is used, the pair-distribution function of the noninteracting gas does not depend on r_s. The explicit dependence on r_s only appears when Coulomb repulsion is taken into account in the wavefunction.

4.2. Interacting electron gas

The interacting case can now be treated by introducing an effective potential which describes the electron-electron interactions in a uniform electron gas. The spherical Bessel functions j_ℓ which appear in Eqs. (16) and (17) are solution of the noninteracting radial Schrödinger equation

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2 \right] u_\ell = 0 \qquad u_\ell = kr\, j_\ell(kr). \qquad (23)$$

If we introduce an effective radial potential $V(r, r_s)$ which depends on the electron-electron distance r and parametrically on the electron density r_s, we can solve the corresponding interacting radial Schrödinger equation,

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - V(r, r_s) + k^2 \right] u_\ell = 0 \qquad u_\ell = kr\, R_\ell(r, k, r_s). \qquad (24)$$

The radial functions R_ℓ will depend parametrically on k and on r_s. We can insert them into Eqs. (16) and (17), and find the corresponding $g_{\uparrow\downarrow}$ and $g_{\uparrow\uparrow}$:

$$g_{\uparrow\downarrow}(r, r_s) = \sum_{\ell=0}^{\infty} (2\ell+1)\langle R_\ell^2(r, k, r_s)\rangle \qquad (25)$$

$$g_{\uparrow\uparrow}(r, r_s) = 2 \sum_{\substack{\ell=1 \\ \text{odd } \ell}}^{\infty} (2\ell+1)\langle R_\ell^2(r, k, r_s)\rangle. \qquad (26)$$

To compute the average over all the possible relative k (represented again by the symbol $\langle\rangle$) one should in principle use the interacting momentum distribution, which deviates from the Fermi step function of the ideal gas. This would slightly change $p(k)$ of Fig. 1 by adding a "tail" for $k > k_F$ and lowering the maximum. For practical purposes, the use of the noninteracting $p(k)$ is enough to give good results.[14] Notice that unless the potential $V(r, r_s)$ is very sophisticated, the treatment just described will fail to recover the long-range correlations, which are mainly governed by collective modes, and will fail to satisfy the particle-conservation sum rule of Eq. (5).

5. SOLUTION OF THE OVERHAUSER MODEL

In this section, we compute an interacting pair-distribution function following the procedure just described by using the simple model potential $V(r, r_s)$ proposed by Overhauser.[13] This simple model gives very good results for the short-range ($r < r_s$) part of $g(r)$.[14]

5.1. The Overhauser potential

Overhauser[13] proposed a simple and reasonable model for the screened Coulomb repulsion $V(r, r_s)$ in the uniform electron gas: he took the sphere of volume n^{-1} as the boundary within which the screening charge density is ne and outside of which it is zero. We thus have the electrostatic potential due to a point charge $-e$ in the

origin plus a sphere around it of radius r_s and of uniform positive charge density ne. In Hartree atomic units:

$$V(r, r_s) = \frac{1}{r_s}\left(\frac{r_s}{r} + \frac{r^2}{2r_s^2} - \frac{3}{2}\right) \qquad r \leq r_s$$

$$V(r, r_s) = 0 \qquad r > r_s. \qquad (27)$$

This is equivalent to assuming that in the interacting gas the probability of finding three electrons in a sphere of radius r_s is exactly zero, an assumption which is nearly true. In fact, numerical estimates of this probability for the electron gas show that it is indeed small.[15] (At $r_s = 5$ the ratio between the probabilities of finding three and two electrons in the same sphere of radius r_s is about 1/11; for larger r_s this ratio is lower, and for smaller r_s it is higher, being about 1/7 at $r_s = 0$.) Thus, for interelectronic distances $r < r_s$ we expect the Overhauser potential to be close to the true potential felt by an electron moving in a uniform electron gas when another electron is fixed at the origin. In the region $r > r_s$ the potential is set to zero, and so is not expected to be reliable. We also expect to have results that become more accurate as the density decreases, since the probability of having three electrons in the same sphere of radius r_s becomes lower and lower. Finally, at high and intermediate densities our results will be much closer to the true $g(r)$ for antiparallel-spin correlations than for parallel-spin ones. When two electrons of opposite spins are in the same sphere of radius r_s, a third electron is excluded from the sphere because of both the Pauli principle and the Coulomb repulsion. For a pair of parallel-spin electrons, only the Coulomb repulsion prevents a third electron of opposite spin from entering the sphere of radius r_s, a mechanism which becomes less efficient as the density (and thus the kinetic energy) increases.

5.2. Solution of the model

The radial Schrödinger equation corresponding to the Overhauser potential can be solved analytically (but not in closed-form),[14] and the functions $R_\ell(s, q, r_s)$ (where $s = r/r_s$ and $q = kr_s$ are scaled variables) are found. As an example, in the left panel of Fig. 2, the radial functions corresponding to $r_s = 4$, $\ell = 0$, and three different values of the scaled relative momentum $q = kr_s$ are reported, together with the effective potential. For an unpolarized uniform gas, the probability distribution for q can be obtained from Eq. (18) by setting $k_F = \frac{1}{r_s}(\frac{9\pi}{4})^{1/3}$,

$$p(q) = \frac{16}{3\pi}q^2\left[2 - \left(\frac{12}{\pi}\right)^{1/3}q + \frac{4}{9\pi}q^3\right], \qquad (28)$$

with q ranging from 0 to $(9\pi/4)^{1/3} \approx 1.91916$. This $p(q)$ is exact for a noninteracting gas. As said, $p(q)$ for the interacting gas slightly deviates from Eq. (28), and depends explicitly on r_s. However, in the region where the potential is reliable, $r/r_s \leq 1$, we see from Fig. 2 that the q-dependence of R_ℓ is very weak, as already pointed out by Overhauser.[13] We thus expect to have no significant change in the short-range ($r < r_s$) part of g if we use an interacting momentum distribution instead of Eq. (28).

In the right panel of Fig. 2 the $g(r)$ obtained by solving the Overhauser model are reported, and compared with the newest diffusion Quantum Monte Carlo (QMC)
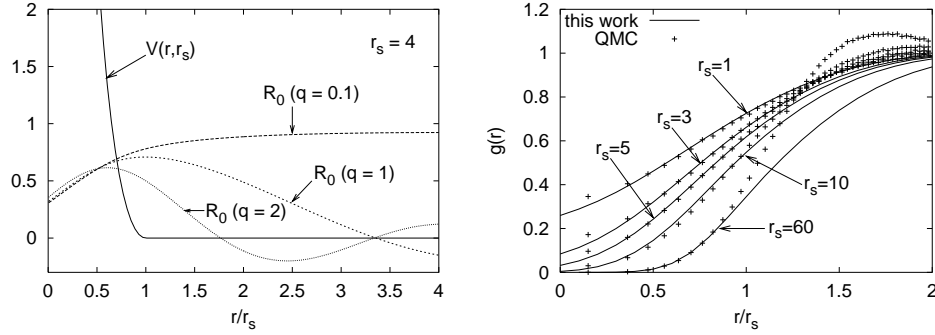
Figure 2: Left panel: the Overhauser potential $V(r, r_s)$ for $r_s = 4$, together with the radial wavefunctions $R_{\ell=0}$ for different values of the scaled relative momentum $q = kr_s$. Right panel: pair-distribution functions $g(r)$ of jellium computed with the Overhauser potential compared to the Quantum Monte Carlo data of Ortiz, Harris and Ballone.[16]

data of Ortiz, Harris, and Ballone.[16] In the range $0 \leq r/r_s \leq 2$, a truncation of the infinite sum over ℓ in Eqs. (25) and (26) at $\ell_{max} = 7$ is enough to reach good convergence.[14] We see that there is accurate agreement with the QMC data for $0.5 \lesssim r/r_s \lesssim 1$ for a wide range of electron densities. In the shortest-range region, $r/r_s \lesssim 0.5$, the QMC data are known to suffer large errors and are not so reliable. (In this region there is in fact a significant discrepancy between the data from Ref. 16 and those from Ref. 17.) Thus, for $r/r_s \lesssim 0.5$ the present treatment should provide results much closer to the true $g(r)$. As said, for $r/r_s > 1$ the results obtained with the Overhauser potential are not reliable.

6. SUMMARY AND CONCLUSIONS

Two-electron wavefunctions (geminals) for the uniform electron gas of density $n = 3/4\pi r_s^3$ are found using the simple screened Coulomb potential proposed by Overhauser. These wavefunctions give pair-densities in agreement with the QMC simulations in the short-range ($r < r_s$) region. They should thus be accurate for $r < r_s$, and could be used as a comparison for other two-electron approaches to the jellium model, and for testing reduced-density matrix energy functionals. In particular, it would be of great interest to compare them with the geminals which will be computed following the approach described by P. Ziesche in this book.

The main lack of the present treatment is the violation of the particle-conservation sum rule. A possible solution to this problem is to write down a self-consistent set of equations in which the effective potential is unknwon, but the "exact" pair-density of jellium[18, 19] is used to generate it.

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